Perfluorotriethylamine 359-70-6 | DTXSID40189464

359-70-6	DTXSID401	894

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: -0.00180

Global applicability domain: Inside

Local applicability domain index: 8.36e-01

Confidence level: 5.39e-01

Nearest Neighbors from the Training Set

Image not found

Methane

Measured: -0.380 Predicted: 1.72e-03 Image not found

Ethylene

Measured: 0.28

Predicted: 4.19e-01

Image not found

Carbon tetrafluoride Measured: -0.950 Predicted: -0.359

Image not found

Ethane

Measured: 0.42 Predicted: 1.04 Image not found

Chloromethane Measured: 1.39 Predicted: 1.58